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Performance assessment of Cu_2SnS_3 (CTS) based thin film solar cells by AMPS-1D

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ABSTRACT

A relative performance assessment of copper tin sulfide (CTS) thin film solar cells with different phases such as, cubic, tetragonal, and orthorhombic as an absorber layer has been carried out by AMPS-1D simulation software. Based on the proposed device architecture, the effects of thickness and carrier concentration for the absorber layer as well as the back metal contact with various work function are studied in order to improve the performance of CTS solar cell. It is found that 10^{18} cm^{-3} and 2500 −3000 nm are optimum values for carrier concentration and thickness for all the investigated CTS absorber layer phases, respectively. On the other hand, back contact metal work function of 5.28 eV, 5.67 eV and 5.71 eV are identified to be the optimal values for cubic, tetragonal, and orthorhombic phases, respectively. We have analyzed in detail the output performance of CTS thin film solar cell with respect to its fabrication, which can serve a constructive research pathway for the thin film photovoltaic industry.

1. Introduction

The urgency in enhancing power conversion efficiency (PCE) and lowering the overall production cost of solar photovoltaic modules has never been greater due to the alarming global warming phenomena induced by a decade of fossil fuel usage. Though the crystalline silicon based solar cells (heterojunction back-contact type) have demonstrated the highest PCE of 26.7% (single cell designated area: 79.0 cm^2) and 24.4% (module designated area (108 cells): 13177 cm^2) [1] among the wafer based technologies, thin film solar cell technology offers a greater advantage in terms of reduced consumption of raw material, exclusion of energy intensive manufacturing process and higher performance stability at practical operating temperature. Chalcogenide based cadmium telluride (CdTe) and copper indium gallium selenide (CIGS) are the two leading second generation thin film photovoltaic technologies, which have presented highest PCE of 22.1% and 22.6%, correspondingly [1]. However, due to the incorporation of toxic (Cd) and comparatively scarce (Te, In) elements, there exist a few shortcomings in terms of the overall sustainability of these technologies if they are to play a central role in global electricity generation in multi-terawatt (TW) scale [2–4]. In the last 3 decades, earth abundant and environmentally friendly copper zinc tin sulfoselenide (CZTSSe) kesterite based pentanary photovoltaic material and thin film solar cell have undergone rigorous research as it is poised to be the successor of the well-established CIGSSe based photovoltaic technology. However, pure sulfide, pure selenide and sulfoselenide based devices have recorded highest PCE of 11.0%, 9.8%, and 12.6% in laboratory scale so far, which are well below the pre-commercialization enabling efficiency benchmark of 15% [5–7].

One of the main PCE retarding features of CZTSSe photoabsorber material is the facile formation of donor-acceptor [Cu_{Zn} + Zn_{Cu}] defect complex. Cu_{Zn} anti-site defect induces deleterious deep acceptor level in the band gap and subsequently deteriorates the device performance through Fermi-level pinning mechanism [8,9] crystal structures, which results in potential fluctuations in the electronic band structure, consequently

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decreasing the effective band gap energy as well as lowering the open circuit voltage (V_{oc}) [10–12]. Thus, considering at the current rapidity of enhancement in the PCEs of CZTSSe based devices, which is constrained by the aforementioned detrimental intrinsic defects, an alternative material with relatively similar abundancy and non-toxicity is highly sought. Copper tin sulfide (CTS) ternary compound is one of the notable secondary phases, which forms during fabrication process of CZTS absorber layer through the intermixing of binary compounds of CuS and SnS. CTS exhibits photovoltaic desirable optoelectronic properties such as p-type conductivity with very high absorption coefficient (10^5 cm^{-1}) along with optimal band gap range (0.9–1.6 eV) [13–16]. Furthermore, the constituent elements of CTS are also non-toxic and earth abundant similar to CZTS. However, due to the absence of Zn, the synthesis process and compositional controllability of CTS are expected to be comparably easier than CZTS. More importantly, with the absence of Zn in CTS material system, the unfavorable [$Cu_{Zn} + Zn_{Cu}$] defect complex can be completely avoided, hence an enormous renewed interest is shown by the photovoltaic research community to explore the properties of CTS as an absorber layer [16]. Kuku and Fakulujo reported the first CTS based thin film solar cell with PCE of 0.11%, which was fabricated by direct evaporation method [15]. Currently, the record PCEs for CTS based solar cells are 4.6% (Na doped CTS) [17] and 6% (Ge alloyed CTS-CTGeS) [18], indicating that the progress towards high efficiency photovoltaic device is still in its embryonic stage. As an inevitable result of polymorphic nature of CTS compound, various phases of CTS such as hexagonal, cubic, tetragonal, monoclinic, triclinic and orthorhombic are reported so far [16,19–21]. These phase variations are due to the possible deviation from the octet rule, which states that formation of compound with the lowest energy level is possible if the total sum of valence electrons of cations surrounding the anion divided by coordination number (for tetrahedral bonded CTS, coordination number is four) plus anion valence electron number is equal to eight. For CTS, there are five tetrahedral coordination possibilities for anion (S), such as: Cu_4, Cu_3Sn, Cu_2Sn_2, $CuSn_3$, and Sn_4. However, none of them satisfies the octet rule [21], which indicates that to form a charge neutral CTS compound, only Cu_2Sn_2 and Cu_3Sn clusters can exist surrounding the anion atoms with 1:2 ratio. The well-defined short-range order stables the compound, while long-range disorder results in the formation of different phases in CTS. The structural and the associated compositional variations in each of these phases are expected to induce different wave-orbital overlapping and splitting mechanisms, which ultimately results in the observed wide-range varying electronic band structure and concomitant optoelectronic properties such as band gap, absorption coefficient and electron affinity [16,19,22].

Since optoelectronic properties of photo-absorbing layer are crucial in determining PCE, the primary objective of this study is to assess the performance of thin film solar cells, which employs various phases of CTS ternary compound as absorber layer by numerical simulation. Physical, optoelectronic and electrical CTS parameters such as layer thickness, energy band gap, electron affinity, absorption coefficient, and carrier concentration are varied, and the resulting changes in V_{oc}, short circuit current density (J_{sc}), fill factor (FF) and PCE (η) are recorded and plotted in the form of 2D performance contours. Initial numerical investigation on the effects of different back contact metals on the performance of CTS devices are also studied with the aim of identifying an optimal back contact metal for different phases of CTS compound. The overall prospects and shortcomings of CTS thin film solar cell are assessed based on the photovoltaic performance parameters obtained numerically herein.

2. AMPS-1D modelling and CTS thin film device structure

In this simulation study, AMPS-1D (Analysis of Microelectronic and Photon Structures) software is used to simulate and compare the performance of CTS based solar cells. AMPS-1D is a computer oriented simulation program, which was developed in 1999 by Stephen Fonash et al. of Pennsylvania State University, USA [23]. This one dimensional device simulation computer program is capable of replicating the working mechanism of homojunction, heterojunction, multijunction and Schottky barrier based solar cell device structures, and it is used by various research groups worldwide [24]. AMPS-1D employs finite differences and Newton-Raphson iteration techniques to solve the one dimensional Poisson's equation for electric field along with continuity equations for holes and electrons. With the proper use of this simulator, a wide range of photovoltaic performance parameters and charge carrier profiles such as V_{oc}, J_{sc}, FF, PCE, spectral response (SR), and charger carrier generation and recombination profiles can be precisely obtained upon numerical convergence [25].

Substrate type device structure of Al/n-ZnO:Al/i-ZnO/n-CdS/p-CTS/Mo/SLG as shown in Fig. 1 is employed here, and the choice of heterojunction device stack configuration is predominantly determined by the well-established technological feasibility and proven successes in CIGSSe and CZTSSe solar cells [7,26].

Hence, this aforementioned structure is adopted in this numerical study, which consists of soda lime glass (SLG) as a substrate, molybdenum (Mo) as a back contact, CTS as a p-type absorber layer, cadmium sulfide (CdS) as a n-type buffer layer, intrinsic zinc oxide (i-ZnO) as a highly resistive transparent window (HRT) layer, aluminium doped ZnO (ZnO:Al) as a transparent conducting oxide (TCO) layer, and finally Al as a front contact metal layer. Relative accurateness of simulated results ultimately depends on the numerical values of CTS material parameters that are inputted in AMPS-1D software. Hence, stringent selection of CTS material parameters based on available literature and several assumptions are made in order to ensure that the obtained simulation outcome is a proper reflection of practicability of CTS compounds as an absorber layer in the proposed thin film photovoltaic architecture. The fundamental physical and electrical parameters for each layer as well as the interfacial contact properties of front (Al/Al doped ZnO) and back (CTS/Mo) metal-semiconductor junctions used in our simulation are listed in the following Table 1 and rationalization for the choice of selected parameters are discussed herein.

Numerical values of all the parameters for ZnO:Al and CdS layers

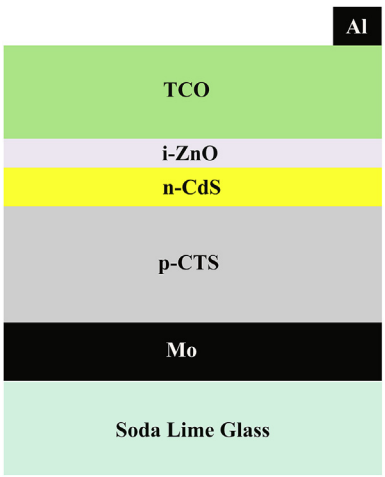

Fig. 1. Substrate type CTS device stack configuration.

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